Lecture 25: Worked Examples

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Application in Statistical Mechanics

Consider the exponential probability distribution

$$f(x) = \begin{cases} \lambda\ e^{-\lambda x} & x \geq 0 \\ 0 & x < 0 \end{cases} \qquad (\lambda > 0)$$

Compute its Fourier transform and verify your answer by an inverse

Solution

The forward transform of the distribution

$$\tilde{f}(k) = \int_0^\infty \lambda\ e^{-\lambda x}\ e^{-ikx}\ \mathrm{d}x = \frac{\lambda\ e^{(-ik-\lambda)x}}{(ik+\lambda)}\bigg|_\infty^0 = \frac{\lambda}{\lambda + ik}$$

can also be interpreted as

$$\tilde{f}(k) = \langle e^{-ikx} \rangle = \left\langle \sum_{n=0}^{\infty} \frac{(-ikx)^n}{n!} \right\rangle = \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} \langle x^n \rangle$$

giving us a mean formula: $\langle x^n \rangle = \dfrac{\mathrm{d}^n}{\mathrm{d}(-ik)^n} \tilde{f}(k)\bigg|_{k=0} \equiv \displaystyle\int_0^\infty x^n\ f(x)\ \mathrm{d}x$

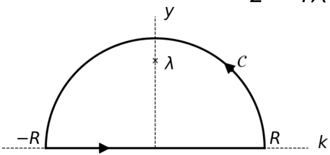
Function Recovery

Reverse transform is given as

$$f(x) = \frac{\lambda}{2\pi}\int_{-\infty}^{\infty} \frac{e^{ikx}}{\lambda + ik}\,\mathrm{d}k = \frac{\lambda}{2\pi i}\int_{-\infty}^{\infty} \frac{e^{ikx}}{k - i\lambda}\,\mathrm{d}k$$

To use complex integration, set $z = k + iy$ and take $g(z) = \dfrac{e^{izx}}{z - i\lambda}$

The residue at $z = i\lambda$, yields



$$\frac{\lambda}{2\pi i}\oint_{\mathcal{C}} g(z)\,\mathrm{d}z = \lambda e^{-\lambda x}$$

$$\lambda e^{-\lambda x} = \lim_{R\to\infty} \frac{\lambda}{2\pi i}\left[\int_{-R}^{R} \frac{e^{ikx}}{k - i\lambda}\,\mathrm{d}k + \int_{0}^{\pi} \underbrace{\frac{e^{ixR\cos\theta - xR\sin\theta}\; iRe^{i\theta}}{Re^{i\theta} - i\lambda}}_{\sim e^{-xR\sin\theta} \to 0}\,\mathrm{d}\theta\right]$$

Yielding us $\boxed{\lambda\, e^{-\lambda x} = f(x)}$

Application in Quantum Mechanics

The wavefunction of a free electron in one dimension is given by

$$f(x) = \left(\frac{1}{2\pi\sigma^2}\right)^{1/4} e^{-x^2/4\sigma^2} \, e^{ik_0 x}$$

Get the probability distributions in position and momentum spaces

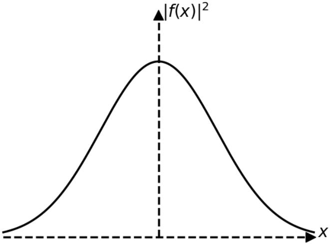
Solution

Notice that $f(x)$ is a complex quantity, but its *norm square*

$$|f(x)|^2 = \left(\frac{1}{2\pi\sigma^2}\right)^{1/2} e^{-x^2/2\sigma^2} \text{ is real}$$

$$\equiv \text{ probability distribution}$$

$|f(x)|^2$ peaks at $x = 0$ "most likely position"



Probability Distribution in x-space

The electron is *somewhere* in the position x-space

$$\int_{-\infty}^{\infty} |f(x)|^2 \, dx = \int_{-\infty}^{\infty} \left(\frac{1}{2\pi\sigma^2} \right)^{1/2} e^{-x^2/2\sigma^2} \, dx = 1$$

Only normalized wavefunctions can represent a physical particle

Probability of finding the e^- near some x_0 is $|f(x_0)|^2 \, dx$

Q. What about momentum space?
A. To seek this, we invoke the De-Broglie's hypothesis,

$$p = \frac{h}{\lambda} = \frac{h}{2\pi} \frac{2\pi}{\lambda} = \hbar k$$

Thus momentum space is the k-space, and we therefore need

$$\tilde{f}(k) = \int_{-\infty}^{\infty} f(x) \, e^{-ikx} \, dx$$

Momentum k-space

$$\begin{aligned}
\tilde{f}(k) &= \int_{-\infty}^{\infty} \left(\frac{1}{2\pi\sigma^2}\right)^{1/4} e^{-x^2/4\sigma^2}\, e^{i(k_0-k)x}\, \mathrm{d}x \\
&= \left(\frac{1}{2\pi\sigma^2}\right)^{1/4} \int_{-\infty}^{\infty} e^{-[x-i(k_0-k)2\sigma^2]^2/(4\sigma^2)}\, e^{-(k-k_0)^2\sigma^2}\, \mathrm{d}x \\
&= \left(\frac{1}{2\pi\sigma^2}\right)^{1/4} e^{-(k-k_0)^2\sigma^2} \underbrace{\int_{-\infty}^{\infty} e^{-[x-i(k_0-k)2\sigma^2]^2/(4\sigma^2)}\, \mathrm{d}x}_{\text{Gaussian Integral}} \\
&= \left(\frac{1}{2\pi\sigma^2}\right)^{1/4} e^{-(k-k_0)^2\sigma^2}\, (4\pi\sigma^2)^{1/2}
\end{aligned}$$

where the Gaussian integral is easily solved* by contour integration

*Refer appendix

Probability Distribution in k-space

From $\tilde{f}(k)$, we obtain

$$|\tilde{f}(k)|^2 = (8\pi\sigma^2)^{1/2} \; e^{-2(k-k_0)^2\sigma^2}$$

We can now invoke the Parseval's theorem

$$\boxed{\frac{1}{2\pi}\int_{-\infty}^{\infty} |\tilde{f}(k)|^2 \, \mathrm{d}k = 1 = \int_{-\infty}^{\infty} |f(x)|^2 \, \mathrm{d}x}$$

The e^- has some momentum, and is somewhere on the x-axis

The momentum probability distribution is therefore, $\dfrac{|\tilde{f}(k)|^2}{2\pi}$

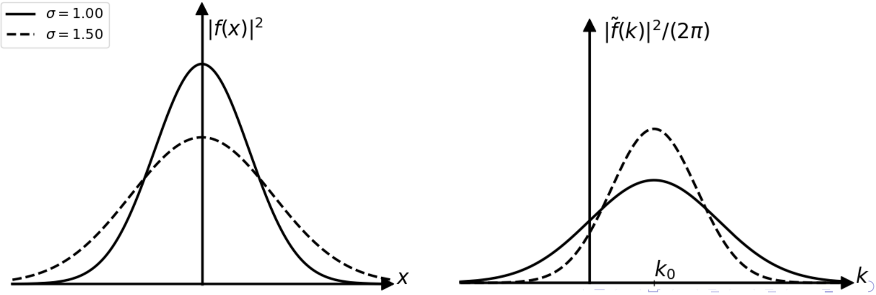
Probability of finding the e^- near some $p_0 = \hbar k_0$ is $\dfrac{|\tilde{f}(k_0)|^2}{2\pi}\,\mathrm{d}k$

Uncertainty Principle

The probability distributions derived so far,

$$\frac{|\tilde{f}(k)|^2}{2\pi} = \left(\frac{2\sigma^2}{\pi}\right)^{1/2} e^{-2(k-k_0)^2\sigma^2} \qquad |f(x)|^2 = \left(\frac{1}{2\pi\sigma^2}\right)^{1/2} e^{-x^2/2\sigma^2}$$

- Fourier transform of a Gaussian is another Gaussian
- Phase factor of e^{ik_0x} in $f(x)$ shifts the center of $|\tilde{f}(k)|^2$ to k_0
- Product of variances, $\boxed{\sigma_k^2\,\sigma_x^2 = \text{const}}$ Uncertainty Principle



N-dimensions

Fourier transforms are easily generalized to N-dimensions, say 3D

$$\begin{aligned}\tilde{f}(\mathbf{k}) &= \int_{V(\mathbf{r})} f(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{r}}\, \mathrm{d}^3\mathbf{r} \\ f(\mathbf{r}) &= \frac{1}{(2\pi)^3} \int_{V(\mathbf{k})} \tilde{f}(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{r}}\, \mathrm{d}^3\mathbf{k}\end{aligned}$$

Fourier transforming the unity

$$\int_{V(\mathbf{r})} e^{-i\mathbf{k}\cdot\mathbf{r}}\, \mathrm{d}^3\mathbf{r} = (2\pi)^3\, \delta^3(\mathbf{k}) \qquad \int_{V(\mathbf{k})} e^{i\mathbf{k}\cdot\mathbf{r}}\, \delta^3(\mathbf{k})\, \mathrm{d}^3\mathbf{k} = 1$$

$$\int_{V(\mathbf{k})} e^{-i\mathbf{k}\cdot\mathbf{r}}\, \mathrm{d}^3\mathbf{k} = (2\pi)^3\, \delta^3(\mathbf{r}) \qquad \int_{V(\mathbf{r})} e^{i\mathbf{k}\cdot\mathbf{r}}\, \delta^3(\mathbf{r})\, \mathrm{d}^3\mathbf{r} = 1$$

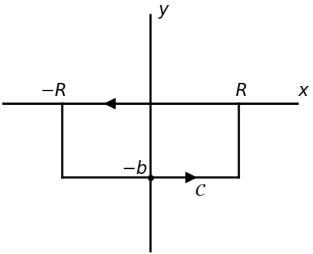
where the 3D δ-distributions in $\mathbf{r}$- and $\mathbf{k}$-space are respectively

$$\begin{aligned}\delta^3(\mathbf{r}) &= \delta(x)\, \delta(y)\, \delta(z) \\ \delta^3(\mathbf{k}) &= \delta(k_x)\, \delta(k_y)\, \delta(k_z)\end{aligned}$$

Appendix

Evaluate $\mathcal{I} = \int_{-\infty}^{\infty} e^{-(x-ib)^2/(4\sigma^2)}\,\mathrm{d}x \qquad b = (k_0 - k)2\sigma^2 > 0$

Solution



Consider $z = x + iy$ and the function

$f(z) = e^{-z^2/(4\sigma^2)}$ and the loop $\mathcal{C}$

$$\begin{aligned}
\oint_{\mathcal{C}} f(z)\,\mathrm{d}z &= 0 \\
&= \int_{-R}^{R} e^{-(x-ib)^2/4\sigma^2}\,\mathrm{d}x + \int_{-b}^{0} e^{-(R+iy)^2/(4\sigma^2)}\,\mathrm{d}(iy) \\
&+ \int_{R}^{-R} e^{-x^2/4\sigma^2}\,\mathrm{d}x + \int_{0}^{-b} e^{-(-R+iy)^2/(4\sigma^2)}\,\mathrm{d}(iy)
\end{aligned}$$

As $R \to \infty$, the y-integrals vanish as the integrands $\sim e^{-R^2}$, giving

$$\boxed{\mathcal{I} = \sqrt{4\pi\sigma^2}}$$